Exercise 8

For the hydrogen atom, if $\int |u|^2 \, d\mathbf{x} = 1$ at $t = 0$, show that the same is true at all later times. (*Hint:* Differentiate the integral with respect to t, taking care about the solution being complex valued. Assume that u and $\nabla u \to 0$ fast enough as $|\mathbf{x}| \to \infty$.)

Solution

Following the hint, differentiate the given integral with respect to time. Note that because u is complex, $|u|^2 = u\bar{u}$, where $\bar{u}$ is the complex conjugate of u.

$$\frac{d}{dt} \int_{\text{all space}} |u|^2 \, d\mathbf{x}$$

$$\frac{d}{dt} \int u\bar{u} \, d\mathbf{x}$$

$$\int \frac{\partial}{\partial t}(u\bar{u}) \, d\mathbf{x}$$

$$\int (u_t\bar{u} + u\bar{u}_t) \, d\mathbf{x} \tag{1}$$

The Schrödinger equation for the hydrogen atom is given as

$$-ihu_t = \frac{h^2}{2m}\Delta u + \frac{e^2}{r}u.$$

If we take the complex conjugate of both sides, we get the differential equation satisfied by $\bar{u}$.

$$\overline{-ihu_t} = \overline{\tfrac{h^2}{2m}\Delta u + \tfrac{e^2}{r}u}$$

$$ih\bar{u}_t = \frac{h^2}{2m}\Delta\bar{u} + \frac{e^2}{r}\bar{u}$$

If we substitute u_t and $\bar{u}_t$ into (1), we get

$$\int \left[\frac{1}{-ih}\left(\frac{h^2}{2m}\Delta u + \frac{e^2}{r}u\right)\bar{u} + \frac{u}{ih}\left(\frac{h^2}{2m}\Delta\bar{u} + \frac{e^2}{r}\bar{u}\right)\right] d\mathbf{x}.$$

Simplifying gives

$$\frac{1}{ih}\int \left(-\frac{h^2}{2m}\Delta u\bar{u} - \cancel{\frac{e^2}{r}u\bar{u}} + \frac{h^2}{2m}u\Delta\bar{u} + \cancel{\frac{e^2}{r}u\bar{u}}\right) d\mathbf{x}$$

$$\frac{h}{2mi}\int (u\Delta\bar{u} - \bar{u}\,\Delta u)\, d\mathbf{x}. \tag{2}$$

Here we invoke Green's second identity, which says that

$$\iiint_D (u\Delta v - v\Delta u)\, d\mathbf{x} = \oiint_{\text{bdy } D} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right) dS$$

for any pair of functions, u and v. This is covered in section 7.2 of the book. For this problem, $v = \bar{u}$. Hence, (2) becomes

$$\frac{h}{2mi} \oiint_{\text{bdy space}} \left(u \frac{\partial \bar{u}}{\partial n} - \bar{u} \frac{\partial u}{\partial n} \right) dS.$$

Recall that $\partial u / \partial n = \mathbf{n} \cdot \nabla u$ is the directional derivative in the outward normal direction, where $\mathbf{n}$ is the unit outward normal vector on the boundary. Since $u \to 0$ and $\nabla u \to 0$ as $|\mathbf{x}| \to \infty$, the integrand becomes 0.

$$\frac{h}{2mi} \oiint_{\text{bdy space}} \left(\underbrace{u}_{=0} \frac{\partial \bar{u}}{\partial n} - \bar{u} \underbrace{\frac{\partial u}{\partial n}}_{=0} \right) dS$$

Therefore,

$$\frac{d}{dt} \int_{\text{all space}} |u|^2 \, d\mathbf{x} = 0,$$

and

$$\int_{\text{all space}} |u|^2 \, d\mathbf{x} = 1$$

for all time.